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- Spectral Shock capturing Techniques
- Parallel Psuedospectral Methods
- Spurious Frequencies in Wake Flows
- Collocation methods based on Wavelets
- Study of High Order Finite Differences and Spectral Methods.
- Hierarchical optimization
- ENO Schemes

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13. ABSTRACT (Maximum 200 words) Research has been carried on the following subjects: <ul style="list-style-type: none"> ° Spectral Shock Capturing Techniques ° Parallel Psuedospectral Methods ° Spurious Frequencies in Wake Flows ° Collocation Methods Based on Wavelets ° Study of High Order Finite Differences and Spectral Methods ° Hierarchical Optimization ° ENO Schemes Summary of the results is presented.				
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Spectral Shock capturing Techniques

The effort to use spectral methods to simulate flows with shock waves is summarized in four published papers. In ([2]) the authors study uniform high order spectral methods to solve multi-dimensional Euler equations for gas dynamics. Uniform high order spectral approximations with spectral accuracy in smooth regions of solutions are constructed by introducing the idea of the Essentially Non-Oscillatory (ENO) polynomial interpolations into the spectral methods. Based on the new approximations, nonoscillatory spectral methods which possess the properties of both upwinding difference schemes and spectral methods were proposed. Numerical results are presented for the inviscid Burger's equation, and for one dimensional Euler equations including the interactions between a shock wave and density disturbance, Sod's and Lax's shock tube problems, and the blast wave problem. Finally, the interaction between a Mach 3 two dimensional shock wave and a rotating vortex is simulated.

In [3] we proved the existence of one-sided filters, for spectral Fourier approximations of discontinuous functions, which can recover spectral accuracy up to the discontinuity from one side. We also used a least square procedure to construct such a filter and test it on several discontinuous functions numerically.

This paper was the prelude to the full solution of the Gibbs phenomenon, the start of it given in the following two papers: It is well known that the Fourier series of an analytic and periodic function, truncated after $2N + 1$ terms, converges exponentially with N , even in the maximum norm. It is also known that if the function is not periodic, the rate of convergence deteriorates; in particular, there is no convergence in the maximum norm, although the function is still analytic. This is known as the Gibbs Phenomenon. In [4] we show that the first $2N + 1$ Fourier coefficients contain enough information about the function, so that an exponentially convergent approximation (in the maximum norm) can be constructed. The proof is a constructive one and makes use of the Gegenbauer polynomials $C_n^\lambda(x)$. It consists of two steps. In the first step we show that the first coefficients of the Gegenbauer expansion (based on $C_n^\lambda(x)$ for $0 < n < m$) of any L_2 function can be obtained, within

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exponential accuracy, provided that both λ and m are proportional to (but smaller than N). In the second step we construct the Gegenbauer expansion based on $C_n^\lambda(x)$, from the coefficients found in the first step. We show that this series converges exponentially with N , provided that the original function is analytic (though periodic). Thus we prove that the Gibbs phenomenon can be completely overcome. Further work had been done in [5]. In this paper we discuss the wave-resolution properties of the Fourier approximations of a wave function with discontinuities. It is well known that a minimum of two points per wave is needed to resolve a periodic wave function using Fourier expansions. For Chebyshev approximations of a wave function, a minimum of points per wave is needed. Here we obtain an estimate for the minimum number of points per wave to resolve a discontinuous wave based on its Fourier coefficients. In our recent work on overcoming the Gibbs phenomenon, we have shown that the Fourier coefficients of a discontinuous function contain enough information to reconstruct with exponential accuracy the coefficients of a rapidly converging Gegenbauer expansion. We therefore study the resolution properties of a Gegenbauer expansion where both the number of terms and the order increase.

Parallel Psuedospectral Methods

We were concerned with the use of parallel computers for spectral methods. For that we have checked Domain Decomposition techniques. In [6] We have outlined a methodology for parallizing spectral methods. The influence of interface boundary conditions on the ability to parallelize pseudospectral multidomain algorithms is investigated. Using the properties of spectral expansions, a novel parallel two-domain procedure is generalized to an arbitrary number of domains each of which can be solved on a separate processor. This interface boundary condition considerably simplifies influence matrix techniques.

These techniques had been improved in [7]. A domain decomposition method is examined to find a time dependent parabolic equation. The method employs an orthogonal polynomial collocation technique on multiple subdomains. the subdomain interfaces are approximated with the aid of a penalty method. The time discretization is implemented in an explicit/implicit finite difference method. The subdomain interface is approximated using an explicit Dufort Frankel method while the interior of each subdomain is approximated using an implicit backwards Euler's method. The principal advantage to the method is the direct implementation on a distributed computing system with a minimum of interprocessor communication. Theoretical results are given for Legendre polynomials while computational results are given for Chebyshev polynomials. Results are given for both a single processor computer and a distributed computing system.

In [8] a method is examined to approximate the interface conditions for Chebyshev polynomial approximations to the solutions of parabolic problems, and a smoothing technique is used to calculate the interface conditions for a domain decomposition method. The method uses a polynomial of one less degree than the full approximation to calculate the first derivative so that interface values can be calculated by using only the adjacent subdomains. Theoretical results are given for the consistency of the scheme and practical results are presented. Computational results are given for a fourth order Runge-Kutta method in two dimentions and compuational results are given for an explicit/explicit scheme in both one and two dimentions.

Spurious Frequencies in Wake Flows

This is an example that a good computation can point out problems in wind tunnel experiments. In [9] A detailed numerical study of two-dimensional flow past a circular cylinder at moderately low Reynolds numbers has been conducted using three different numerical algorithms for solving the time-dependent compressible Navier-Stokes equations. It was found that if the algorithm and associated boundary conditions were consistent and stable, then the major features of the unsteady wake were well predicted. However, it was also found that even stable and consistent boundary conditions could introduce additional periodic phenomena reminiscent of the type seen in previous wind-tunnel experiments. However, these additional frequencies were eliminated by formulating the boundary conditions in terms of the characteristic variables. An analysis based on a simplified model provides an explanation for this behaviour.

Further study of the effect of boundary conditions had been carried out in [1]. The stability theory for finite difference Initial Boundary-Value approximations to systems of hyperbolic partial differential equations states that the exclusion of Eigenvalues and generalized eigenvalues is a sufficient condition for stability. The theory, however, does not discuss the nature of numerical approximations in the presence of such eigenvalues. In fact, as was shown previously [9], for the problem of vortex shedding by a 2-D cylinder in subsonic flow, stating boundary conditions in terms of the primitive (non-characteristic) values may lead to such eigenvalues causing perturbations that decay slowly in space and remain periodic time. Characteristic formulation of the boundary conditions avoided this problem. In this paper, we reported on a more systematic study of the behavior of the (linearized) one-dimensional gas dynamic equations under various sets of oscillation-inducing "legal" boundary conditions.

Collocation methods based on Wavelets

We were the first to try to construct differentiation matrices by wavelets. In [10] Lee Jameson discussed the notion of differentiation matrices. The numerical solution of a partial differential equation requires an easily manipulated spatial approximation to the derivative of the unknown function as well as some method to march forward in time. In general one starts from given values of the unknown function, then a finite dimensional approximation, based on those values, is constructed. This approximation is differentiated and the result are read at the gridpoints. For example, in the pseudospectral Chebyshev method for the discretization of the equation

$$\frac{\partial U(x,t)}{\partial t} = \frac{\partial F[U(x,t)]}{\partial x}$$

One assumes that at a given time the values of $U(x_j, t)$ are given for some points $x_j = \cos(\frac{\pi j}{N})$, ($j = 0, N$). Then one constructs the interpolation polynomial through those points and differentiate *this polynomial* to get approximate values for $\frac{\partial F[U(x,t)]}{\partial x}$ at the point x_j . this procedure can be viewed as a transformation from N given values (of the function) to new N values (approximating the derivative). This is the Chebyshev *Differentiation Matrix*. The numerical algorithm therefore is simple and the boundary conditions can be easily applied. It is natural to ask whether one gain by using wavelets instead of Chebyshev polynomials. . Since wavelets are well localized functions it is reasonable to conjecture that they might represent steep gradients or the development of a shock with a relatively small number of terms. consider a periodic function $f(x)$ given on an equally spaced mesh. Expand it in wavelet expansion and use the derivative of this expansion as an approximation to the derivative of $f(x)$. Lee Jameson, has proved that approximation of a periodic function $f(x)$ in a wavelet basis and the differentiation of this approximation *yields nothing more than a finite difference approximation to a derivative*. The following is an outline of the proof:

i) Given a periodic function $f(x)$ let \vec{s} represent the periodic scaling function coefficients of this function on the finest scale. This requires approximating the inner product of $f(x)$ with the scaling function on the finest scale. The matrix representation of this approximation is circulant in form: $C : \vec{f} \rightarrow \vec{s}$, where \vec{f} represents $f(x)$ sampled on an evenly spaced grid.

ii) Let D be the mapping from the scaling function coefficients of $f(x)$ to the set of scaling function coefficients that represents the derivative of $f(x)$: $D : \vec{s} \rightarrow \vec{\dot{s}}$. Since $f(x)$ is periodic then the matrix form of D is circulant in form.

iii) All circulant matrices of the same size commute, therefore we can apply the operator D directly to \tilde{f} . The operator D has the effect of a finite difference operator, and the proof will be complete.

Therefore, the effect of first approximating in a wavelet basis, then differentiating in this basis and finally converting back from the wavelet basis to the original function is equal to applying the appropriate finite difference operator directly to the equally spaced sampled values of the original function $f(x)$. The proof provides an insight into the possibility of using wavelets for solutions of PDE's.

Wavelets while not more than known finite difference schemes can provide a mechanism for automatic adaptation of the mesh.

In [11] an effort to use Galerkin procedure had been examined for the Bergers equation using wavelets based on splines.

Study of High Order Finite Differences and Spectral Methods.

Several issues concerning the applications of high order methods were examined. In [12] we outlined the direction of the numerical simulations of the next decade and the typical problems associated with large scale computing.

In [13] we examined the way to impose compatibility conditions in Chebyshev methods. Often, in solving an elliptic equation with Neumann boundary conditions, a compatibility condition has to be imposed for well-posedness. This condition involves integrals of the forcing function. When pseudospectral Chebyshev methods are used to discretize the partial differential equation, these integrals have to be approximated by an appropriate quadrature formula. The Gauss-Chebyshev (or any variant of it like the Gauss-Lobatto) formula cannot be used here since the integrals under consideration do not include the weight function. A natural candidate to be used in approximating the integrals is the Clenshaw-Curtis formula; however, we show in this article that this is the wrong choice and it may lead to divergence if time-dependent methods are used to march the solution to steady state. We develop, in this paper, the correct quadrature formula for these problems. This formula takes into account the degree of the polynomials involved. We show that this formula leads to a well conditioned Chebyshev approximation to the differential equations and that the compatibility condition is automatically satisfied

In [14] We study the stability of spectral approximations to scalar hyperbolic initial-boundary value problems with variable coefficients. Time is discretized by explicit multi-level of Runge-Kutta methods of order 3 (forward Euler time differencing is included), and we study spatial discretizations by spectral and pseudospectral approximations associated with the general family of Jacobi polynomials. We prove that these fully explicit spectral approximations are stable provided their time-step, Δt , is restricted by the CFL-like condition, $k \Delta t \leq 1$ where N equals the spatial number of degrees of freedom. We give two independent proofs of this result, depending on two different choices of appropriate ℓ^p -weighted norms. In both approaches, the proofs hinge on a certain inverse inequality interesting for its own sake. Our result confirms the commonly held belief that the above CFL stability restriction, which is extensively used in practical implementations, guarantees the stability (and hence the convergence) of fully-explicit spectral approximations in the non-periodic case.

In [15] we discuss a new type of schemes: In a previous paper we have presented a new method of imposing boundary conditions in the pseudospectral Chebyshev approximation of a scalar hyperbolic equation. The novel idea of the new method is to collocate the equation at the boundary points as well as in the inner grid points, using the boundary conditions as penalty terms. In this paper we extend the above boundary treatment to the case of general constant coefficients hyperbolic systems of equations, and we provide error estimates for the pseudospectral Legendre method. The same scheme can be implemented also in the general (even nonlinear) case.

In [16] A competitive algorithm, which allows the computation of approximated polynomial solutions of advection-diffusion equations in the square, is presented. The equation is collocated at a special grid and the corresponding system is solved by a low-cost preconditioned iterative procedure. The method provides accurate results even when the solution presents sharp boundary-layers.

In [17] The authors examine pseudospectral matrices. A standard way to approximate the solution of differential problems by algebraic polynomials, is to use collocation methods based on nodes related to Jacobi polynomials such as Chebyshev or Legendre polynomials. The matrices corresponding to the classical differential operators are known to be full, non-symmetric and ill-conditioned. We examine those relative to the discretization of Neumann problems in one space dimension. In particular, we are concerned with their approximation properties, their eigenvalues and the possibility to find appropriate preconditioners. Several choices are available when imposing boundary conditions in the approximate problem. For instance, they can be either directly enforced or imposed in a variational way. This results in different behaviors, which can drastically affect the numerical effect of the matrices. We analyze the different cases, pointing out the advantages and drawbacks in using each strategy.

A particular attention is paid to the study of preconditioning matrices.

In [18] a polynomial approximation of functions of matrices is considered. In solving a mathematical problem numerically, we frequently need to operate on a vector by an operator that can be expressed as $f(A)$, where A is a matrix [e.g. $\exp(A)$, A^{-1}]. Except for very simple matrices, it is impractical

to construct the matrix $f(A)$ explicitly . Usually an approximation to it is used. This paper develops an algorithm based upon a polynomial approximation to $f(A)$. First the problem is reduced to a problem of approximating $f(z)$ by a polynomial in z , where z belongs to a domain D in the complex plane that includes all the eigenvalues of A . This approximation problem is treated by interpolating $f(z)$ in a certain set of points that is known to have some maximal properties. The approximation thus achieved is "almost best." Implementing the algorithm to some practical problems is described. Since a solution to a linear system, an iterative solution algorithm can be based on a polynomial approximation to f . We give special attention to this important problem.

In [19] We study several algorithms for computing the Chebyshev spectral derivative and compare their roundoff error. For a large number of collocation points, the elements of the Chebyshev differentiation matrix, if constructed in the usual way, are not computed accurately. A subtle cause is found to account for the poor accuracy when computing the derivative by the matrix-vector multiplication method. Methods for accurately computing the elements of the matrix are presented and we find that if the entries of the matrix are computed accurately, the roundoff error of the matrix-vector multiplication is as small as that of the transform-recursion algorithm. Furthermore, results of the CPU time usage are shown for several different algorithms for computing the derivative by the Chebyshev collocation method for a wide variety of two dimensional grid sizes on both an IBM mainframe and a Cray 2 computer. We find that which algorithm is fastest on a particular machine depends not only on the grid size, but also on small details of the computer hardware as well. For most practical grid sizes used in computation, the even-odd decomposition algorithm is found to be faster than transform-recursion method.

In [20] The stability characteristics of various fourth- and sixth order spatial operators are assessed using the theory of Gustafsson, Kreiss, and Sundstrom (G-K-S) for the semi-discrete Initial Boundary Value Problem (IBVP). These results are then generalized to the fully discrete case using a recently developed theory of Kreiss. In all cases, favorable comparisons are obtained between G-K-S theory, eigenvalue determination, and numerical simulation. The conventional definition of stability is then sharpened

to include only those spatial discretizations that are asymptotically stable (bounded, Left Half Plane eigenvalues). It is shown that many of the higher-order schemes which are G-K-S stable are not asymptotically stable. A series of compact fourth and sixth-order schemes, which are both asymptotically and G-K-S stable for the scalar case, are then developed.

Hierarchical optimization

Prof. Berger started to develop an optimization component in our program. In [21] The idea of hierarchical gradient methods for optimization is considered. It is shown that the proposed approach provides powerful means to cope with some global convergence problems characteristic to the classical gradient methods. Concerning global convergence problems, four topics are addressed: The detour "effect" , the problem of multi-scale problems, the problem of highly ill-conditioned objective functions, and the problem of local-minima traps related to ambiguous regions of attractions.

The great potential of hierarchical gradient algorithms is revealed through a hierarchical Gauss-Newton algorithm for unconstrained nonlinear least-squares problems. The algorithm, while maintaining super-linear convergence rate like the common conjugate - gradient or quasi-Newton methods, requires the evaluation of partial derivatives with respect to only one variable on each iteration. This property enables economized consumption of CPU time in case the computer codes for the derivatives are intensive CPU consumers, e.g., when the gradient evaluations of ODE or PDE models are produced by numerical differentiation.

The hierarchical Gauss-Newton algorithm is extended to handle interval constraints on the variables and its effectiveness demonstrated by computational results.

ENO schemes

In [22], we have performed a comprehensive numerical study regarding the accuracy and convergence of ENO (essentially non-oscillatory) schemes on model problems. We proposed a modified ENO scheme, with no additional computational costs, which can enhance the accuracy in smooth regions. The behavior of the modified ENO scheme near shocks is similar to the original ENO schemes.

In [23], we have applied high order ENO schemes to two and three dimensional compressible Euler and Navier-Stokes equations. Practical issues, such as vectorization, efficiency of coding, cost comparison with other numerical methods, and accuracy degeneracy effects, are discussed. Numerical examples are provided which are representative of computational problems of current interest in transition and turbulence physics. These require both non-oscillatory shock capturing and high resolution for detailed structures in the smooth regions and demonstrate the advantage of ENO schemes.

In [24] we have proposed a new numerical approach to solve systems of conservation laws of mixed hyperbolic-elliptic type, by a generalization of the hyperbolic flux splitting methods. The possibly elliptic flux is split into a sum of two hyperbolic fluxes with only positive/negative eigenvalues. Upwinding hyperbolic solvers can thus be applied to each of them separately. Equipped with time splitting this procedure is stable. Numerical results are shown to illustrate the behavior of this method on the van der Waals equation in gas dynamics. We observe convergence with good resolution to admissible solutions containing phase transitions for Riemann problems. We also tested more general initial conditions.

In [25], we discussed about a framework to use uniformly high order spectral method for solving multi-dimensional Euler equations of compressible flow. Uniform high order approximation with spectral accuracy in smooth regions of the solution is coupled to a non-oscillatory shock transition through the introduction of ENO interpolation idea into the spectral methods. The proposed numerical procedure possesses the properties of both upwinding finite difference schemes and spectral methods. Test problems include Burgers equations, one and two dimensional Euler equations including shock-vortex and shock-wave interactions.

In [26], we discuss the application of high order compact finite difference methods for shock calculations. The main idea is the definition of a local mean which serves as a reference for introducing a local nonlinear limiting to control spurious numerical oscillations while keeping the formal accuracy of the scheme. For scalar conservation laws, the resulting schemes can be proven total variation stable in one space dimension and maximum norm stable in multi space dimensions. Numerical examples are shown to verify accuracy and stability of such schemes for problems containing shocks.

In [27], we applied the discontinuous Galerkin finite element method (the second order version) to 2D Euler equations of gas dynamics. Test problems include the standard shock reflection, backward step problem, and double Mach reflection. Different choices of limiters are explored.

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